Energy Band Structure in Silicon Crystals by the Orthogonalized Plane-Wave Method*

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(Received June 17, 1957)

The values of the energies at the point $K=2\pi a^{-1}(1,0,0)$ are calculated in Si by the orthogonalized plane-wave method. The curves of energy *versus* K are drawn in the [100] direction. The results are in agreement with the fact that Si is an insulator. They also indicate that the minimum of the lowest conduction band lies near the surface of the zone.

THE orthogonalized plane-wave method has proved to be quite accurate in giving the energies of a large number of electronic bands at high symmetry points of the reduced zone.[1] Woodruff[2] has presented the method in a convenient form and has used it to evaluate the energies of the valence and conduction bands in silicon at the point $K=0$ of the reduced zone. In the present work the energy bands have been calculated at the point $K=2\pi a^{-1}(1,0,0)$ by the same method

The sets of plane waves $\langle 100 \rangle$, $\langle 011 \rangle$, $\langle 120 \rangle$, and $\langle 211 \rangle$ have been used in deriving the crystal symmetry combinations of plane waves, which transform according to the irreducible representations of the small group of the wave vector $K=2\pi a^{-1}(1,0,0)$.[3] The approx-

imate atomic-core wave functions and the energy eigenvalues for the Si atom have been evaluated by Woodruff.[2] The coefficients of orthogonality between the plane waves and the core functions are listed in Table I. Since the Fourier coefficients of the potential do not depend on the wave vector K, Woodruff's values of these quantities have been used.

The final results obtained for the energies are presented in Table II. At the point $K=2\pi a^{-1}(1,0,0)$, as at the point $K=(0,0,0)$, the energies of the various states appear in the same order in Si as in diamond.

In Fig. 1 the curves of energy *versus* K are plotted along the [100] axis. The results of Table II and those of Woodruff for the same stage of approximation were used. The interpolation scheme is that proposed by Slater and Koster[4] and the integrals over atomic orbitals are treated as parameters to be fitted to the calculated values of the energies.

From the position of the energy bands in Fig. 1, it can be seen that Si should be an insulator. This was

Table I. Orthogonality coefficients, $A_{nl}(|K+h|)$.[a]

$(a^2/4\pi^2)|K+h|^2$	$A_{1s}(|K+h|)$	$A_{2s}(|K+h|)$	$-iA_{2p}(|K+h|)$
1	0.016941	0.15937	0.045692
2	0.016874	0.14865	0.060936
5	0.016674	0.12142	0.081406
6	0.016608	0.11374	0.084505

[a] $A_{nl}(|K+h|) = (\Omega_0)^{-\frac{1}{2}} \int u_{nl}^* \exp[i(K+h) \cdot r] dv$, where u_{nl} is the core function for the atomic state and Ω_0 is the volume of the unit cell.

Table II. Energies (in rydbergs) of valence and conduction states in Si crystal with $K=2\pi a^{-1}(1,0,0)$.

	$X_1(1)$	$X_4(1)$	$X_1(2)$	$X_3(1)$	$X_4(2)$
E_1[a]	−1.0035	−0.7674		0.2880	
E_2	−1.1153	−0.9464	−0.4547	0.0956	0.4504
E_3	−1.1164	−0.9552	−0.4927		0.2413
E_4	−1.1665		−0.5408		
E_5	−1.1871		−0.5408		

[a] The subscripts attached to E indicate the order of the secular determinant used in obtaining the energies.

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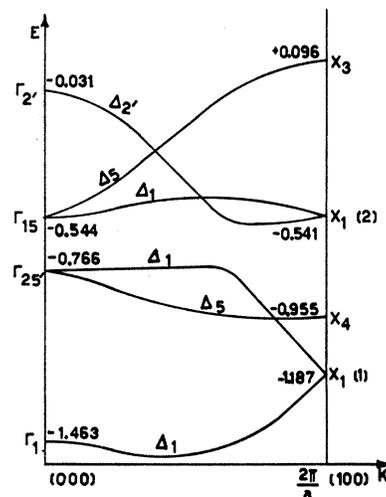
Fig. 1. Diagram of the energy band structure of Si along the [100] axis.

not the case in a recent calculation by Jenkins,[5] who used a variational cellular method. It is difficult to determine the position of the minimum of the conduction bands, because the energies at Γ_{15} and at $X_1(2)$ are almost equal and the interpolation scheme is only approximately valid. Since, however, it has been shown[2] that the value of the energy at Γ_{15} decreases very little if plane waves of higher energy are taken into account,

it is to be expected that the minimum should lie near the point $\mathbf{K} = 2\pi a^{-1}(1,0,0)$, as predicted by Herman.[6]

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Effect of Impurity Scattering on the Magnetoresistance of n-Type Germanium

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(Received June 6, 1957)

Observations in n-type germanium show a decrease in the anisotropy of the magnetoresistance with increased ionized-impurity content and with decreased temperature. Although similar to what is expected due to ionized-impurity scattering, the details of the variation do not agree with calculations assuming anisotropic impurity scattering. Deviations from the magnetoresistance symmetry conditions are observed for crystals with electron concentration $n > 4 \times 10^{15}$ cm^{-3} at 77°K.

THE interpretation[1,2] of magnetoresistance observations[3] in n-type germanium has confirmed the (111) symmetry of the band structure deduced from cyclotron resonance experiments[4,5] at low temperature. However, there is apparent lack of agreement between the anisotropy observed[6–8] in the low-field galvanomagnetic effects and that expected from the cyclotron-resonance effective masses. It has also been observed that the magnetoresistance anisotropy seems to be a function of the concentration of impurities and the temperature at which the measurements were made. In this paper, experimental data pointing out this effect are presented, and possible explanations are discussed.

The magnetoresistance coefficients[3] b, c, and d are defined in Eq. (1). This expression describes the magnetoresistance for a cubic crystal in the low-field region, i.e., where the change in resistivity is proportional to the square of the magnetic field.

$$\frac{\Delta\rho}{\rho H^2} = b + c\frac{(\mathbf{I}\cdot\mathbf{H})^2}{I^2 H^2} + d\frac{\sum_{i=1}^{3} I_i^2 H_i^2}{I^2 H^2}. \quad (1)$$

In this equation ρ is the resistivity, and $\mathbf{I}$ and $\mathbf{H}$ are

the current and magnetic field, with the components taken along the cubic axes. For a conduction-band structure like that in germanium, the coefficients satisfy the conditions:

$$b + c = 0, \quad d > 0. \quad (2)$$

These coefficients are functions of the relaxation time τ and the shape of the energy surfaces, as represented by the ratio of longitudinal to transverse effective masses, K_m. If a specific form is assumed for the dependence of τ on energy, K_m can be calculated directly from the magnetoresistance. If, in addition to the magnetoresistance, the Hall coefficient R and the conductivity σ are known, K_m can be calculated, provided that τ is a function only of the energy of the carriers. Observations of the quantity

$$W \equiv \frac{b + c + d}{b + (R_0\sigma_0)^2} \quad (3)$$

can be used to calculate[9] K from Eq. (4).

$$W = 2\left(\frac{K^2 - 2K + 1}{2K^2 + 5K + 2}\right). \quad (4)$$

Here K is the ratio of the mass anisotropy K_m to the relaxation-time anisotropy K_τ. The latter is defined as the ratio of longitudinal to transverse scattering times in the same directions as the mass ellipsoids. If τ is a

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